

Final Report
5th CHEMICAL CONGRESS OF NORTH AMERICA
CANCUN – November 11–15, 1997

SYMPOSIUM #532: *Laser Control of Electrons and Molecules*

Jeffrey L. Krause
Principal Investigator

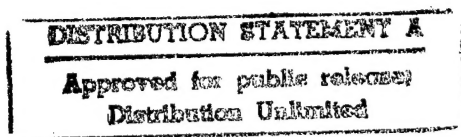
INVITED SPEAKERS

CANADA

A. Bandrauk (Sherbrooke)
P. Brumer (Toronto)
P. Corkum (Ottawa)
D. Miller (Toronto)
T. Nguyen Dang (Laval)
A. Stolow (Ottawa)

USA

P. Bucksbaum (Michigan)
Y. Chen (Berkeley)
R. Coalson (Pittsburgh)
M. Dantus (Michigan State)
L. Dimauro (Brookhaven)
R. Gordon (Illinois)
E. Grant (Purdue)
J. Krause (Florida)
K. Kulander (Livermore)
H. Metiu (Santa Barbara)
K. Nelson (MIT)
H. Rabitz (Princeton)
D. Reitze (Florida)
S. Rice (Chicago)
K. Wilson (San Diego)



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INTRODUCTION

The Fifth Chemical Congress of North America was held November 11-15, 1997, in Cancun, Mexico. This was a major international meeting, sponsored by the American Chemical Society (ACS), the Canadian Society for Chemistry (CSC) and the Sociedad Química de México (SQM). The Federación Latinoamericana de Asociaciones Químicas (FLAQ) was also an official participating organization of the Congress. There were 100 symposia scheduled at the Congress, in thirteen topical areas. Approximately 1700 invited or contributed talks and posters were presented at the meeting.

SYMPOSIUM ON QUANTUM CONTROL

The PI and Prof. André Bandrauk co-organized one of the symposia at the Chemical Congress, entitled "Laser Control of Electrons and Molecules". This symposium was one of the most comprehensive and influential meetings of the year in the rapidly evolving area of quantum control. We asked 21 scientists from Canada and the US to give invited talks at the symposium, all of whom enthusiastically accepted. The list of speakers represents most of the major contributors to the field in North America. We were especially excited that in a field traditionally dominated by theorists, over half of the participants in the symposium are experimentalists. Talks were scheduled over two days, in three four-hour sessions. A list of speakers and the titles of their presentations is attached. Also attached are copies of the abstracts from the Abstract Book for the meeting.

INVITED SPEAKERS AND TITLES

A.D. Bandrauk (Sherbrooke)

Laser Phase Control of Vibrational and Electron Excitations.

P. Brumer (Toronto)

Laser Control of Photodissociation, Bimolecular Processes and Refractive Indices.

P.H. Bucksbaum (Michigan)

Ultrafast probes of Molecular Dynamics.

Y. Chen (Berkeley)

Strong Field Control of Photochemistry.

R.D. Coalson (Pittsburgh)

Laser Control of Electron Transfer.

P.B. Corkum (Ottawa)

Molecular Optics.

M. Dantus (Michigan State)

Laser Control of Bimolecular Reactions.

L.F. Dimauro (Brookhaven)

Long Wavelength Field Induced Dynamics.

R.J. Gordon (Illinois)

Controlling Chemical Reactions by Quantum Interference.

E.R. Grant (Purdue)

Vibrational Control of Electron Ejection in Radicals.

J.L. Krause (Florida)

Quantum Control of Rydberg Wave Packets.

K.C. Kulander (Livermore)

Two-Phase Control of Electron and Proton Emission in H_2^+ .

H. Metiu (Santa Barbara)

Coherent Processes in Quantum Wells.

R.J.D. Miller (Toronto)

Femtosecond Studies of Electron Dynamics at Surfaces.

K.A. Nelson (MIT)

Optical Control of Collective Material Behavior.

T.T. Nguyen-Dang (Laval)

Wave Packet Control of Dissociative Ionization.

H. Rabitz (Princeton)

Altering the Course of Quantum Dynamics.

S.A. Rice (Chicago)

STIRAP Based Active Control of Reactions.

D.H. Reitze (Florida)

Quantum Control of Electronic Charge.

A. Stolow (Ottawa)

Molecular Wave Packet Methods.

K.R. Wilson (San Diego)

Controlling the Future of Matter.

2255.

THERMODYNAMIC APPROACH TO CRACKED-POLYMER VAPOR DEPOSITION (CP-VD).
MIHAI SCARLETE NICOLE SCHMITT, Department of Chemistry, Bishop's University
Lennoxville, Canada, J1M 1Z7

Following the current interest in the use of thin SiC films in the semiconductor silicon growth industry (ref.1,2) as well as new major advancements in the design of heterojunction electronic devices that include dielectric or semiconductor ceramic layers, increased effort is addressed to the design of new deposition methods adapted to increasingly specific requirements. Situated at the midpoint between Chemical Vapor Deposition and Spin Coating of Polymeric Precursors, Cracked-Polymer Vapor Deposition is offered as a possible solution that offers the advantage of high deposition rates of smooth ceramic film on complicated-shaped substrates. Important control parameters are presented for this method, previously used to produce ceramic coatings on various substrates (ref 3). Ref: 1) M. Scarlete in J.Eich.Soc., 1992, 139, 1207. 2) T. Fukuda et al in J.Electrochem.Soc. 1994, 141, 2216. 3)M.Scarlete, I.S.Butler and J.F.Harrod in Can.Ceramic.

Symposium on Laser Control of Electrons and Molecules (532)-Oral

167. ALTERING THE COURSE OF QUANTUM DYNAMICS. H. Rabitz, Department of Chemistry, Princeton University, Princeton, New Jersey, U.S.A., 08544

Efforts at achieving the active manipulation of quantum dynamics are receiving increasing attention. By the introduction of coherent optical fields, it is possible to alter the pathway of molecular dynamics in the most intimate fashion. Establishing this capability could have a number of applications, including manipulating chemical reactions or the creation of unusual dynamical states. The underlying physical principles for quantum dynamical control will be discussed, along with recent developments towards the design of robust controls and the manipulation of atomic translational motion.

168. Ultrafast Probes of Dynamics in Molecules in the Far Infrared and Extreme Ultraviolet P.H. Bucksbaum,^{1,2} J. Caraher,¹ F. Weihe,² C. Raman,¹ J. Yukich,^{1,2} D. Garzella,³ P. Agostini,³ R. Gordon,⁴
¹Physics Department, University of Michigan, Ann Arbor, MI 48109-1022, ²Center for Ultrafast Optical Science, Ann Arbor, MI 48109-2099, ³CEA-Saclay, 91191 Gif-sur-Yvette, France, ⁴Chemistry Department, Univ. of Illinois at Chicago, Chicago, IL.

Atomic motion within excited molecules can be observed using two new ultrafast optical probes: sub-picosecond Half-cycle pulses (HCP), which can map the momentum distribution of loosely bound electrons; and sub-picosecond High Harmonic pulses (HHP) which can probe the charge density near the tightly bound core electrons. These two methods provide different and complementary information about the evolution of a molecule during excitation and dissociation.

169. OPTICAL CONTROL OVER COLLECTIVE MATERIAL BEHAVIOR. Ciaran J. Brennan, Timothy Crimmins, Richard Koehl, and Keith A. Nelson, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02162, USA

Coherent optical control over collective material behavior and structure has been a long-standing objective of ultrafast spectroscopy¹. We report significant progress toward that objective. It is now possible to generate large-amplitude collective motions in condensed materials with single or multiple femtosecond pulses. Recent examples and applications will be discussed. Control capabilities are enhanced by femtosecond pulse shaping methods through which a single incident laser beam consisting of a single femtosecond pulse is transformed into an output laser beam consisting of a pulse sequence or waveform which may be used for enhanced control over material responses, or into many output beams, each of which consists of a different, independently specified waveform and each of which may be directed toward a different region of a sample. Control over both position-dependent and time-dependent material responses will be discussed.

1. Y.-X. Yan, E.B. Gamble, Jr., and K.A. Nelson, J. Chem. Phys. 83, 3591 (1985).

170.

MOLECULAR WAVEPACKET METHODS

Valerie Blanchet & Albert Stolow, Steacie Institute for Molecular Sciences, National Research Council of Canada, 100 Sussex Dr., Ottawa, Ontario K1A 0R6 CANADA

Wavepacket are well known for investigating the short-time classical-like behaviour of molecular excited states. Wavepacket pump-probe measurements are isomorphic with two-photon coherent control experiments and, from this point of view, have presented robust demonstrations of optical phase control. Wavepacket techniques and methods of analysis, both now well established, could be considered together as a general and flexible methodology to be applied to a variety of practical problems. We discuss the isomorphism between wavepacket methods and coherent phase control scenarios and consider several examples of wavepacket methods applied to problems such as laser isotope separation, terahertz switching using wavepacket interferometry and the enhancement of molecular Rydberg lifetimes.

171. LASER CONTROL OF BIMOLECULAR REACTIONS; EXPERIMENTS AND THEORY. M. Dantus, Department of Chemistry, Michigan State University, East Lansing, Michigan 48824, USA.

Bimolecular reactions are characterized by the energy of collision, orientation between reactants and impact parameter. We have developed a novel technique to control these reaction parameters as well as determining the time at which the reaction occurs, without the need for van der Waals precursors. The method used is femtosecond photo-association spectroscopy (FPAS), whereby an ultrafast laser pulse causes binding between free atoms or molecules. U. Marvet and M. Dantus, Chem. Phys. Letters 345, 393 (1995). Results will be shown for different atom+atom and atom+molecule reactions. Wave packet simulations taking into account the incoherent sum of continuum states in the free to bound transition will also be presented. The simulations confirm the coherent bond formation processes.

172. VIBRATIONAL CONTROL OF ELECTRON EJECTION IN POLYATOMIC FREE RADICALS, E. E. Mayer, E. J. Zückerman, J. M. Behm, H. G. Hedderich and E. R. Grant, Department of Chemistry, Purdue University, West Lafayette, IN 47906

Photoselection via double resonance excites specific vibrational modes in selected high-Rydberg states of polyatomic free radicals such as HCO, NO₂ and CH₃CO. Total energy in these systems exceeds lowest ionization potentials, enabling neutral molecules to decay by vibrational relaxation coupled with electron ejection (vibrational autoionization). Relaxation rates determine homogeneous linewidths of individual rovibronic resonances. These linewidths reflect a mode specificity that varies with the degree of anharmonic vibrational coupling in the core. Trends in general fit with expectations based on Multichannel Quantum Defect Theory extended to the multidimensional vibrational space of polyatomic molecules.

173. **CONTROLLING THE FUTURE OF MATTER.** *K. R. Wilson*, Department of Chemistry and Biochemistry, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0339

I will show theoretical and experimental examples of quantum control; placing atoms where we want them with desired momentum at a time of our choosing, as well as control of electron dynamics, with a long term goal of controlling chemical bonding. Experiments in our lab demonstrate such wavepacket focusing, the control of nuclear quantum dynamics with tailored ultrafast pulses of light in both gas and condensed phases. In addition, transient quantum nano- and picostructures can be produced which can in turn be used to programmably control by interference and diffraction the distributions of light and matter in space and time.

For more complex systems where, for example, we don't know the detailed nature of the potential surfaces, feedback control will be necessary, in which the experimental progress with respect to the goal (for example a particular chemical reaction) is measured and the tailoring of the driving light field is iteratively optimized. I will illustrate progress in implementing an "ideal" measurement, ultrafast x-ray diffraction and spectroscopy.

669. **LASER CONTROL OF PHOTODISSOCIATION, BIMOLECULAR PROCESSES AND REFRACTIVE INDICES.** *P. Brumer*, Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Canada M5S 3H6

The principle of coherent radiative control of molecular processes is simple: by coherently driving a pure molecular state through multiple optical excitation routes to the same final state one can introduce laboratory controllable quantum interference terms. Manipulating these laboratory parameters then allows for selective control over desired molecular properties. In this talk we describe recent advances, including the use of lasers to control the photodissociation of Lithium dimer, to affect bimolecular reactions and to modify refractive indices of gases.

670. **CONTROLLING CHEMICAL REACTIONS BY QUANTUM MECHANICAL INTERFERENCE.** Langchi Zhu, Kunihiro Suto,* Jeanette Allen Fiss, Ryuichi Wada,* and Robert J. Gordon, Department of Chemistry (m/c 111), University of Illinois at Chicago, 845 W. Taylor St., Chicago, IL 60607

In a recent publication (L. Zhu et al., *Science* 270, 77 (1995)) we reported the coherent phase control of the competition between photoionization and photodissociation of HI molecules. Control was achieved by absorption of three photons of frequency ω , and one photon of frequency $\omega_3=3\omega$, just above the first ionization threshold. The product signals were modulated by varying the phase difference between the two laser beams. These signals displayed a phase lag which depended on the excitation energy. We now show that the energy dependence of the phase lag is caused by a resonance state of the parent molecule coupled to two continua. This phase lag has a deep minimum at the center of the resonance and rises monotonically on either side. The possible role of the "molecular phase" of the product wave functions will be discussed.

- 670a. **Coherent processes involving electrons in quantum wells: optical excitations and transport.**

by *Horia Metiu* and *Pablo Tamborenea*
Department of Chemistry and Physics and
The Center for Quantum Electronic Structures
University of California, Santa Barbara, CA 93106

By solving exactly the time dependent Schrodinger equation we study a variety of optical and transport processes involving a dilute electron gas in several quantum well structure. The main theme is electron coherence induced by a strong laser and its effect on the transport properties of the mesoscopic structure. We discuss laser induced localization, wave packet interferometry and negative resistance.

671. LASER CONTROL OF CONDENSED PHASE ELECTRON TRANSFER. Rob D. Coalson, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260 USA, and Yuri Dakhnovskii, Department of Chemistry, University of Antioquia, AA 1226, Medellin, COLOMBIA

A theory of laser induced perturbation of electron transfer systems strongly coupled to a condensed phase environment will be presented. It will be shown that the rates of electron transfer between donor and acceptor site can be strongly modified by application of an appropriate light field, as can the long-time distribution of donor/acceptor populations [J. Chem. Phys. **103**, 298 (1995)]. A way of switching population using picosecond light pulses is suggested [Phys. Rev. Lett. **75**, 3649 (1995)]. The optical absorption spectrum of such systems (e.g., mixed valence transition metal complexes in polar solvents) under high intensity irradiation will also be discussed [Phys. Rev. Lett. **77**, 2917 (1996), J. Chem. Phys. **105**, 9441 (1996)].

671a.

QUANTUM CONTROL OF RYDBERG WAVE PACKETS. Jeffrey L. Krause, Quantum Theory Project, University of Florida, Gainesville, FL 32611, and Kenneth J. Schafer, Department of Physics, Louisiana State University, Baton Rouge, LA 70803.

Ultrafast laser pulses can be used to create shaped Rydberg wave packets with structures on the nanometer length scale. Experimental detection of these structures is complicated because they form near the turning point of the Coulomb potential, where the electron is nearly free. Several detection schemes have been suggested, each of which is sensitive to a different property of the wave packet. Ultrafast diffraction using high order harmonics appears to be an especially promising probe of these transient nanostructures. We present calculated, time-dependent diffraction patterns simulating the expected signal in an experimental measurement. We also discuss extensions to alkali metal atoms, and to control of multidimensional wave packets, localized in both the radial and angular dimensions.

672.

QUANTUM CONTROL OF ELECTRONIC CHARGE IN TAILORED POTENTIALS USING ULTRAFAST LASERS. David H. Reitze, Jeffrey L. Krause, Hyun Yoon, Nicole M. Beach, Chad Hansing, and Ben J. Streetman, Physics Department, University of Florida, Gainesville, FL, 32611

Laser control of charge distributions in chemical potentials is a precursor to the control of chemical reaction pathways. Here, we explore the use of ultrafast laser pulses to control charge motion in an idealized yet experimentally realizable potential, namely, that of a coupled semiconductor quantum well system. In particular, we implement a quantum 'control loop' consisting of an oscillating electronic wave packet in a double quantum well, an optical pulse shaper, and real-time feedback in which the excitation laser pulse is dynamically optimized during the course of the experiment to achieve the target wave-packet state. In addition, we examine the sensitivity of the control loop to external perturbations such as changes in potential shape and wave packet coherence times. Finally, we compare our results with results using quantum optimal control theory.

672a.

FEMTOSECOND STUDIES OF ELECTRON DYNAMICS AT SURFACES: FEASIBILITY OF BALLISTIC ELECTRON PHOTOCHEMISTRY. R. J. Dwyer, Departments of Chemistry and Physics, 60 St. George Street, University of Toronto, Toronto, Canada M5S 1A7.

The coherence in the optical preparation of excited electrons at surfaces is quickly lost through electron-electron and electron-phonon scattering processes. Recently, it has been demonstrated that coherent control of electrons is feasible and optical interference of two different frequency phase related optical fields have been used to generate currents. The question is whether or not the same degree of control can be exercised in terms of photochemical processes involving photoexcited electrons. Femtosecond Photoemission Spectroscopy gives a unique probe of both the dephasing processes in the electronic polarization and the level dynamics to completely describe the electron dynamics at surfaces. Results will be presented for metal and semiconductor single crystal surfaces, for both three dimensional and two dimensional materials. The electron dynamics will be contrasted with the nuclear relaxation and electron transfer dynamics to discrete molecular states at surfaces, using a variety of nonlinear optical probes of surface reaction dynamics. These studies taken together determine the feasibility of exploiting ballistic electrons in surface reaction channels and give an upper limit to the quantum efficiency of hot electron chemistry.

1031. STIRAP BASED ACTIVE CONTROL OF PRODUCT FORMATION IN A REACTION. Stuart A. Rice, The James Franck Institute, The University of Chicago, 5640 South Ellis Ave., Chicago, Illinois 60637

A scheme for active control of product formation in a chemical reaction, based on an extension of STIRAP, will be discussed.

1032. LASER PHASE CONTROL OF VIBRATIONAL EXCITATIONS AND ELECTRON IONIZATION. A.D. Bandrauk, S. Chelkowski and H. Yu. Laboratoire de Chimie Théorique, Faculté des sciences, Université de Sherbrooke, Que, J1K 2R1, Canada.

Two types of phase control will be considered by: 1) chirped single frequency pulses; 2) two colour laser pulses with a different phase ϕ . In the first case it will be shown from a dressed state representation how efficient excitation of symmetric vibrations can be achieved by RCAP - Raman Chirped Adiabatic Passage. The second scheme will be shown to be useful for enhancing high order harmonic generation by molecular ions in order to produce coherent VUV and new X-Ray radiation.

- 1033.

LONG WAVELENGTH LIMIT OF FIELD INDUCED DYNAMICS. L. F. DiMauro, B. Sheehy, Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973, K. C. Kulander, TAMP Group, Lawrence Livermore National Laboratory, Livermore, CA 94551

Over the past decade, there has been a dramatic increase in our understanding of strong-field interactions. Theoretical and experimental advances forged a consistent view of a field-driven electron rescattering with the core producing high energy electrons and photons. Experimentally, the major advance came with the evolution of kilohertz repetition rate laser technology. For the first time, experiments probed regions which revealed the fundamental importance of the rescattering event, as well as raising some intriguing questions about multielectron excitation. Although successful, experimental access is still limited by dynamics dictated by visible or near-visible excitation. In this talk, we will report on our experimental studies which probe field-induced dynamics in the long-wavelength limit, a virtually unexplored regime. This is realized by a newly developed short pulse, tunable mid-infrared (3-5 μm) laser source which maintains the advantage of kilohertz technology. Investigations are now possible which explore the tunneling dynamics of a large number of atomic and molecular systems at large ponderomotive potential.

1034. TWO-COLOR PHASE CONTROL OF THE ELECTRON AND PROTON EMISSION DIRECTIONS IN STRONG FIELD, MULTIPHOTON EXCITATION OF H_2^{+} K.C. Kulander, Lawrence Livermore National Laboratory, PO Box 808, Livermore CA 94551 and F.H. Mies, National Institute for Standards and Technology, Gaithersburg MD 20899

A strong, short-pulsed laser field can cause a molecule to either dissociate or ionize, depending on the partitioning of the absorbed energy between the electronic and nuclear degrees of freedom. If the exciting field is a combination of the laser and its second harmonic with a defined relative phase, control of the direction of the emitted particles becomes possible. Using a collinear model for this system, we can explicitly follow the time-dependent dynamics of the excitation. An asymmetry in the proton directional distribution is created by the two color field. During the asymmetric dissociation the Coulomb explosion of the molecular ion at large R imprints a similar asymmetry in the direction of the emitted electron. This propensity agrees with the recent measurements on HD^+ [B. Sheehy, B. Walker and L. F. DiMauro, PRL 74, 4799 (95)]

*This work was performed in part under the auspices of the U. S. Department of Energy at the Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

1035. WAVEPACKET CONTROL OF THE DISSOCIATIVE IONIZATION OF H_2 IN AN IR LASER FIELD. T. T. Nguyen-Dang and F. Châteauneuf, Dept. de Chimie, Université Laval, Québec, G1K 7P4, Que, Canada.

The dissociation dynamics of H_2^+ in a low-frequency laser field depend critically on the synchronization between the wavepacket motions and those of the time-dependent adiabatic potential energy surfaces. For an appropriate synchronization between the wavepacket preparation and the onset of the field, a dynamical vibrational trapping may occur by a 'clapbox' mechanism. While this effect can easily be understood in a time-dependent wavepacket picture, its Floquet interpretation is not obvious. This interpretation will be discussed with the aim to establish a clearcut distinction between this new, laser-induced, dynamical trapping mechanism and the more well known vibrational trapping effect associated with the Floquet picture. The stability of the new dynamical trapping effect with respect to realistic variations in initial conditions, simulating the continuous preparation of the ionic species by the tunnel ionization of the parent H_2 molecule, is then discussed, through wavepacket calculations that include this continuous ionization as a Feshbach resonance process.

1036. STRONG FIELD CONTROL OF PHOTOCHEMISTRY. Y. Chen, Department of Chemistry, University of California, Berkeley, CA 94720-1460, USA.

We propose a new strategy for laser controlled chemistry. The scheme is based on the temporal modulation of electronic potential surfaces by intense ultrashort laser pulses. In the study of the time resolved photoelectron spectroscopy of nitric oxide (NO), we demonstrated that the Rydberg-valence interaction in NO can be significantly enhanced by an intense femtosecond pulse. The concept is also applied to the study of the photodissociation of OC10 where we have successfully enhanced the product branching ratio of (O2+C1) over (C1O+O) by a factor of 12.

1037. Molecular Optics.

P. B. Corkum, C. Ellert, C. Milne, H. Stapelfeldt, H. Sakai, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Ontario, Canada K1A 0R6.

When intense light interacts with molecules it induces a dipole force through the gradient of the Stark shift. We use this force to deflect I_2 and CS_2 molecules. We trace the direction of molecules in the molecular beam, showing that the molecules that pass through the intensity gradient near the centre of the high intensity region of a 1.06 μm or 10.6 μm laser beam will focus. We predict that Stark shifts on the order of 50 meV can be obtained for all small atoms and molecules while maintaining ionization rates below $10^6 s^{-1}$.

Symposium on Metal Clusters and Metal-Ligand Interactions (585)-Oral

1693. STUDIES ON THE INITIAL CHEMICAL EVENTS IN NITROGEN FIXATION, Krassimir K. Stavrev and Michael C. Zerner, Quantum Theory Project, University of Florida, Gainesville, FL 32611

Nitrogen reacts with protons in the enzyme nitrogenase to form ammonia in one of the most efficient and central processes in biology. Recently the structure of the enzyme has been determined, and the active site seems to be a FeMo-cofactor, a molecule with seven Fe atoms and one Mo atom, bridged by sulfur atoms. We examine this system, and possible reaction sequences that lead to the fixation of nitrogen in an attempt to learn what is so very unique in this system.

Our proposed model for the FeMo-cofactor is consistent with the experimental data available from ESR, Mossbauer and ENDOR spectroscopies. We follow the initial activation of the nitrogen molecule in the cofactor and subsequently model the hydrogenation of N_2 up to the fourth protonation step. The results obtained favor the reaction mechanism going through hydrazido intermediates on the four-Fe surfaces.

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